Numerical Simulations on Propagating Process of $H_2/O_2/H_2O$ Cylindrical Detonation with Detailed Reaction Model

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1 Introduction

Detonation is a supersonic combustion wave propagating with a leading shock wave and flame front in a reactive mixture. The detonations could cause the explosion accidents because of its high temperature and high pressure. Many studies have been carried out for the safety engineering purpose.

On March, 2011, the explosion accident was occurred at the Fukushima nuclear power plant. It is thought as follows that the detonation occurs in nuclear power plants. The fuel-cladding Zircaloy is oxidized by high-temperature steam, and then hydrogen is generated. Reacting hydrogen and oxygen in the air triggered, the deflagration-to-detonation transition(DDT) and the detonation are generated[1]. In order to prevent such an accident, it is necessary to clear the cause of occurence of the DDT and the direct initiation of detonation under high concentration steam condition.

There is considerable investigation on DDT and direct initiation of detonation in the nuclear power plants[2]. It is difficult, however, to clearly understand the phenomenon by only experimental investigation because of the difficulty to measure the detonation propagation with a supersonic speed. If one would find out the cause of DDT and direct initiation of detonation in nuclear power plant, large-scale examination facilities would be necessary and it would requires huge cost and time. Therefore, numerical researches are necessary to find the feature of the DDT and the direct initiation of detonation in a premixed hydrogen/oxygen gas mixture with high-temperature and high-concentration of steam. The present study firstly focuses on the direct initiation of detonation.

In the previous experimental investigations[3,4], it was specified that there are the critical initiation energy for direct initiation of detonation. The numerical study by Eckett et al.[5] demonstrated that the unsteadiness of the induction zone was dominant in the failure of spherical detonation. Watt and Sharpe[6] carried out the two-dimensional simulation to determine the cellular stability. But influences of (i)the atmospheric steam and vapar droplet concentration, and (ii)the critical initiation energy are still not clear.

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The objective of this study is to investigate the critical initiation energy of hydrogen/oxygen/steam cylindrical detonation in unconfined space using the numerical simulation. In the present simulation, latest detailed chemical reaction model UT-JAXA[13] is applied. In this paper, the critical initiation energy of cylindrical detonation at 0% and 10% steam concentration is investigated using one- and two-dimensional simulations.

2 Numerical Method and Simulation Conditions

The governing equations are the compressible Euler equations with a chemically reacting gas system in a one-dimensional cylindrical coordinate system. The time integration method is 3rd-order TVD Runge-Kutta method[8]. For the convective term, the numerical scheme is AUSMDV scheme[7] with 2nd order MUSCL including minmod limiter. The integral approach of reaction source terms is the 5th order backward differentiation formulas. The variable time step is automatically caluculated by VODE code[9], which is based on Gear method[10]. As for the two-dimensional simulations, the time integration scheme and the numerical flux are the same as the one-dimensional simulation. The two-dimensional simulations with fifth-order WCNS(Weighted Compact Nonlinear Scheme) schemes[11,12] also carried out to find out the effect of the spartial resolution. WCNS has the following three advantages compared with WENO:(1) various flux splitting method can be used; (2) interpolation of flow variables can be used despite the finite difference formulation; and (3) free-stream and vortex preservation properties are very good on a wavy grid[12]. Moreover, WCNS can capture shock waves well and increase grid size keeping grid resolution compared with MUSCL. The source term is integrated by the point implicit method to reduce the computational cost.

In the present simulation, the detailed chemical reaction model UT-JAXA[13] containing 8 species (H_2, O_2, H, O, OH, HO_2, H_2O_2 and H_2O) and 21 elementary reactions adopts for high pressure states to solve a cylindrical detonation problem. In this model, a detailed explanation for H_2, O_2, and H_2O reactions is presented. Because third-body efficiencies of these elementary are very important and sensitive to the accuracy of the model under high-pressure and no-diluent conditions.

The initial condition is separated into two computational regions; one is near the center of the cylinder with the source energy and another with the ambient values. The pressure and temperature of source energy region are 100 atm and 2000 K, respectively. The initial energy depends on the radius of the source energy region, which is defined by a radius of the source, r_s. The pressure and temperature of the ambient region are 1 atm and 373.15 K, respectively. The gas in both regions consists of a stoichiometric(Φ= 1) H_2/O_2 gas mixture. The vapor droplets are neglected in this simulations.

For the one-dimensional case of 0% steam concentration, the grid size, Δx, is 2.5 μm, which corresponds to the resolution of 16 grid points in the half reaction length, $L_{1/2}$. The half reaction length is defined as the distance from the shock wave to the place where the mass fraction of hydrogen is equal to the average of the free stream value and the equilibrium steady state value. It is used as length unit. In this ambient condition, $L_{1/2}$, is 40.3 mm. The case of 10% steam concentration, Δx is 2.5 μm, which corresponds to the resolution of 29 grid points in $L_{1/2}$. In this ambient condition, $L_{1/2}$, is 71.3 mm. For the two-dimensional simulations, Δx and Δy are 5 μm in order to reduce computational const. The grid system is the orthonal grid with 2401x2401. The simuation with a higher-resolution grid will be presented in the conference. The radius of ignition source is 0.75 mm.

3 Results and Discussions

Succesfull initiation is defined as the number of oscillations of velocity and pressure is over 2 in this study. The initiation energy depends on r_s. Figures 1 and 2 show the time histories of the detonation velocity and shock pressure under 0% steam concentration for various r_s. r_s is 1, 2, 5 and 10 mm. The broken lines in Figs. 1 and 2 denote the CJ velocity (D_{CJ} = 2818.8 m/s) and the pressure at von Neumann spike (P_{vN} = 2.6 MPa). The one-dimensional cylindrical detonation oscillates around the CJ detonation state and does not continue to propagate at any initial condition. The oscillation is due to the interaction between the leading shock and the combustion front. The number of oscillations of

velocity and pressure is over 2 when r_s = 10 mm. Thus, it is succesfull initiation when r_s = 10 mm. The number of oscillations of velocity is under 2 when r_s = 1, 2, and 5 mm. It is concluded that one-dimensional cylindrical detonation for 0% steam concentration can propagate if r_s is over 10 mm in this initial condition.

Figures 3 and 4 show the time histories of the detonation velocity and shock pressure of 10% steam concentration for various r_s. r_s is 1, 2, 5, 10 and 20 mm. The broken lines in Figs. 3 and 4 denote the CJ velocity (D_{CJ} = 2692.1 m/s) and the pressure at von Neumann spike (P_{vN} = 2.5 MPa). The number of oscillations of velocity and pressure is over 2 when r_s = 10, 20 mm. Thus, it is succesfull initiation when r_s = 10, 20 mm. The number of oscillations of velocity is under 2 when r_s = 1, 2, and 5 mm. It is concluded that one-dimensional cylindrical detonation for 10% steam concentration can propagate if r_s is over 10 mm in this initial condition.

The initiation energy is given by

$$E = \frac{\pi (r_s)^2 p_s}{\gamma - 1}$$

p_s is the pressure in the source energy region, γ is the constant ratio of specific heats in the source energy region[6]. Therefore, initiation energy is approximately 10 kJ/m when r_s = 10 mm, approximately 2.5 kJ/m when r_s = 5 mm. Lee J.H.S. indicated semi-empirical model about the critical initiation energy[4]. According to this model, the critical initiation energy of detonation for 0% steam concentration is approximately 4.3 kJ/m in this condition. Therefore, it seem that the critical initiation energy of detonation for 0% and 10% steam concentration is probably between 2.5 kJ/m and 10 kJ/m.

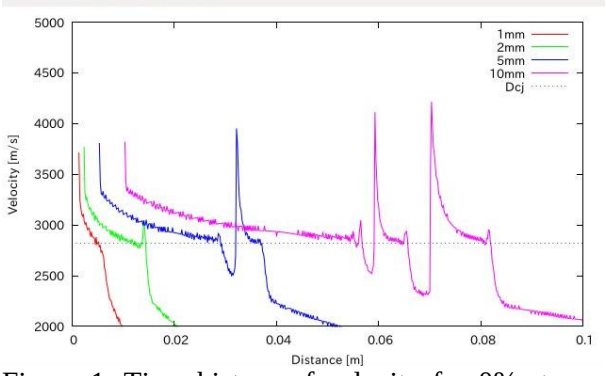


Figure 1. Time history of velocity for 0% steam concentration.

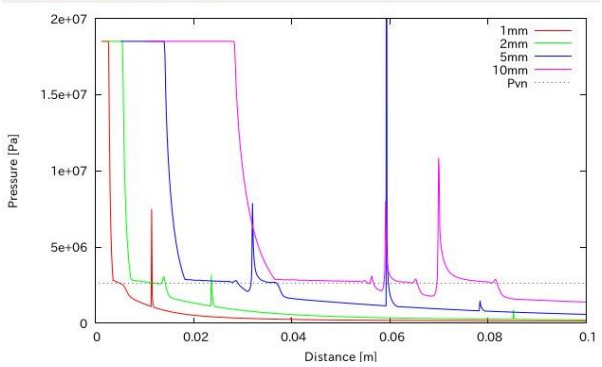


Figure 2. Time history of shock pressure for 0% steam concentration.

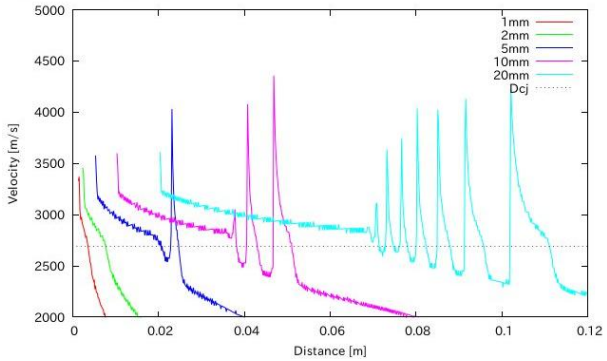


Figure 3. Time history of velocity for 10% steam concentration.

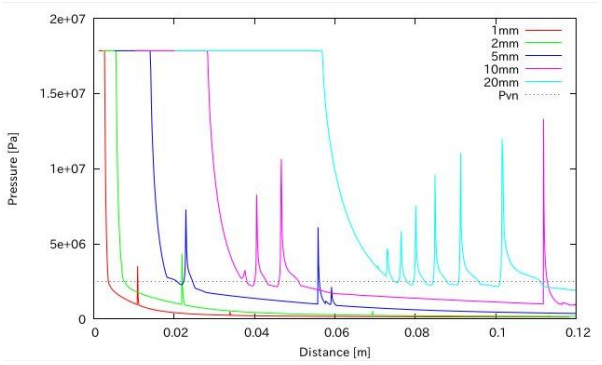
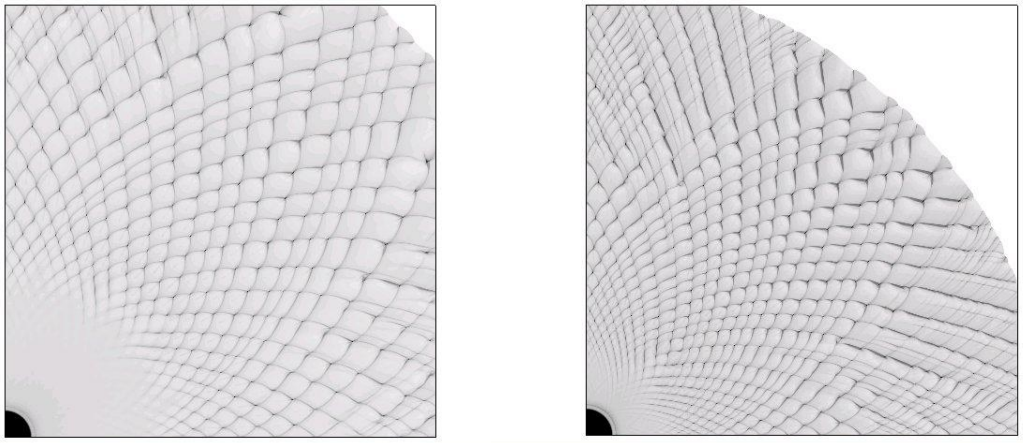


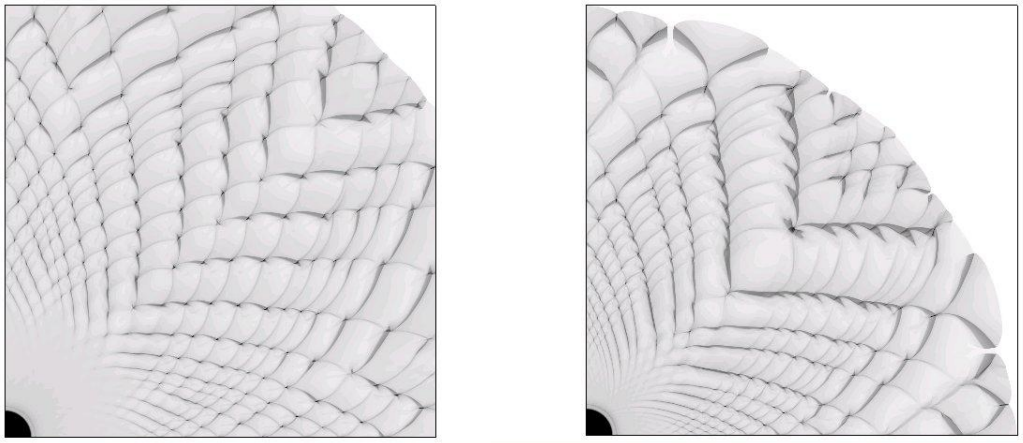
Figure 4. Time history of shock pressure for 10% steam concentration.

Figure 5 shows the maximum pressure histories for 0% stem concentration in the two-dimensional simulations. The cellular structures for both resolutions are regular and the both cell sizes are similar at the same radius location. The cellular structure for WCNS is clearer than that for MUSCL. The cellular structure near the ignition core region can be found for WCNS. Figure 6 shows the maximum pressure histories for 10% stem concentration. Both cellular structures become irregular and the cell sizes increases comparing with the case for 0% stem concentration.



(a)Second-order MUSCL (b)Fifth-order WCNS

Figure 5. Maximum pressure histories for 0% stem concentration.



(a)Second-order MUSCL (b) Fifth-order WCNS

Figure 6. Maximum pressure histories for 10% stem concentration.

4 Conclusions

The one- and two-dimensional cylindrical detonations by the direct initiation were simulated with the detailed chemical reaction model in the stoichiometric H_2/O_2 gas with 0% or 10% steam concentration mixture. As a result of the influences of the initiation energy, the critical initiation energy of detonation for 0% and 10% steam concentration is probably between 2.5 kJ/m and 10 kJ/m when the pressure and temperature of source energy region are 100 atm and 2000 K and those of ambient region are 1 atm and 373.15 K. As for the influences of steam concentration in the two-dimensional simulations, the higher steam concentration requires the higher initiation energy, and the larger cell size and the more irregular cellular structures appear.

Acknowledgments

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